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Notification of SCALE 5 Software Error

An error has been identified in SCALE 5 that may impact certain type of unit cells, specifically asymmetric and symmetric slab cells (ASYMSLABCELL and SYMMSLABCELL). Users are encouraged to follow the checklist below to determine if the error applies to their problems and if the potential impact is non-trivial.

Checklist for *Safety-Significant Software Error* Notification

Item	
Software Identification	SCALE 5, RSICC # CCC-725. (Previous versions are NOT impacted.)
Data Library	N/A
Computing platform (Unix, Windows, Linux, etc.)	All computing platforms
Description of the error	In SCALE 5, the LATTICECELL input format was changed to use keywords. As part of these changes, errors were introduced in the calculation of dimensions for asymmetric and symmetric slab cells. These programming errors in the Materials Information Processor (MIPLIB) cause an inaccurate Dancoff factor calculation from a SCALE 5 control sequence and will cause errors in the predicted k-eff value that uses the Dancoff factor.
How was the error identified?	Y-12 encountered a fatal error when running SCALE 5 with a SCALE 4 input file for a CSAS case that used the ASYMSLABCELL option for a LATTICECELL geometry type. Y-12 sent the file to ORNL to examine and ORNL discovered two programming errors: (1) an error in the conversion of a SCALE 4 input file using ASYMSLABCELL (fatal error, code dies) and (2) an error in the Dancoff factor calculation when the ASYMSLABCELL or SYMMSLABCELL option is used with the new SCALE 5 format.
When does the error occur?	The error only occurs for control sequence input files that use the ASYMSLABCELL or SYMMSLABCELL option and the new SCALE 5 input format (keywords "READ COMP"). If a SCALE 5 control sequence is executed using input files developed with the SCALE 4 format, the input file will not properly convert to a SCALE 5 input format and a fatal error will result before any calculations are performed.
Potential impact of error	The impact of the erroneous Dancoff factor calculation on the system k-eff value is problem dependent. Analyses performed at ORNL indicate that the error in k-eff can be potentially significant if the ASYMSLABCELL option is used. The impact of the error on k-eff is relatively minor for cases where the SYMMSLABCELL option is used. Plate-type fuel is perhaps one of the most common uses for the slab cell option in SCALE and lower enriched systems will

	tend to demonstrate larger errors due to the importance of the Dancoff factor. ORNL used an infinite system of 20% enriched MTR fuel as a sample test. The SYMMSLABCELL case provided a k-inf value that was slightly conservative (~0.8%) in SCALE 5, but the ASYMSLABCELL case yielded a k-inf value that was non-conservative by more than 15%. For high-enriched MTR fuel, the ASYMSLABCELL case was non-conservative by less than 4% and the SYMMSLABCELL case was slightly conservative. The error in k-eff for the ASYMSLABCELL cases shown here are large. However, if a user's application applies the ASYMSLABCELL option and sufficient critical benchmarks with the ASYMSLABCELL are included in the SCALE 5 validation set, then the impact of the error may already be accounted for in the bias and uncertainty applied in the safety case. There is no impact if SCALE 4 input files are used, because those cases will fail during SCALE's automatic conversion of the input to SCALE 5, prior to any calculation.
Frequency / likelihood of error occurring	The ASYMSLABCELL option is seldom used. If users apply an existing SCALE 4 input file with the ASYMSLABCELL option, the code would fail with a fatal error before any calculation is performed. The non-fatal error that yields an incorrect k-eff value can only occur for cases that use the ASYMSLABCELL or SYMMSLABCELL option in the SCALE 5 input format. For cases with the SYMMSLABCELL, the impact of erroneous Dancoff factor on the predicted k-eff is small and not a significant safety concern; however, for cases that use the ASYMSLABCELL option, the erroneous Dancoff factor could potentially produce a significant error in k-eff.
How can users determine if error affects their calculations?	Check for input files that use the keywords ASYMSLABCELL or SYMMSLABCELL and use the SCALE 5 input format (search for the keywords "READ COMP").
What action should users take if error affects them?	Replace the LATTICECELL geometry specification and the ASYMSLABCELL or SYMMSLABCELL input option with an equivalent MULTIREGION geometry specification and a SLAB input option. Tests at ORNL have confirmed that the MULTIREGION specification with the SLAB option will produce the correct prediction of k-eff.
Is correction to code/data available?	The MIPLIB programming will be corrected in SCALE 5.1 (scheduled for release in March 2006).
How to obtain/install correction	If you encounter this problem, contact ORNL at scalehelp@ornl.gov and we will assist you.